United States
Environmental Protection
Agency

ECOTOX Knowledgebase 2024 Training

Worksheet: Example 1

This worksheet was developed for the Workshop session of the ECOTOX Knowledgebase at the in-person NAMs Tools Training Workshop hosted by the U.S. Environmental Protection Agency's Center for Computational Toxicology and Exposure April 24 – 25, 2024.

For more information about the ECOTOX Knowledgebase tool:

- Visit the ECOTOX Knowledgebase at www.epa.gov/ecotox.
- Contact ECOTOX support at ecotox.support@epa.gov or by calling 218-529-5225.
- Read more in Olker et al. 2022, https://doi.org/10.1002/etc.5324.

Goal

Use the ECOTOX knowledgebase to identify and explore records available for specific chemicals, species groups, and other refined searches.

Directions

1. Find the chemical information for DEET from the list provided on page 5 of this worksheet. *[Note: For the first round of this worksheet, we will all start with the chemical DEET. If you have time during or after the training, select another chemical from page 5 to work through on the worksheet.]*

    a. Type the chemical and its CAS Registry Number in the space below.

2. Because we are starting with a chemical and have no other parameters, should you start with Search or Explore?   Answer: Search

        Explore

3. Create a Custom Group for your chemical. *[Hint: Go to Explore, select Chemicals, then create custom group. Enter in your chemical name or CAS Registry Number. Then refer to the list of Query Filters on the left-hand side to walk through the next set of questions.]*

    a. How many Species Groups have records in ECOTOX for the selected compound(s)?

4. Refine these results by selecting the **Fish** Species Group. *[Note: For the first round of this worksheet, we will all start with Fish. If you have time during or after the training, select another species group from page 5 to work through on the worksheet.]*

   a. What changed when you selected the Fish Species Group?

   b. Based on the Species Group you selected, take note that the "Aquatic"/"Terrestrial" options at the top of the left-hand side may change automatically depending on which Species Group(s) are selected. For example, Birds only have Terrestrial data. You can also manually change these selections to narrow results, for example if you only want Terrestrial data for Amphibians (which could have both Aquatic and Terrestrial data). If you are using another species group that has both habitats, select a specific habitat to see how the number of records change.

5. Change the view as needed (i.e., Group Summary, Records, Plot View – icons located above the output table) to answer the following questions:
   a. Change your results to Records view.

      i. What types of effects were investigated in the Species Group you focused on?
      [Again, for this first round of the worksheet, the output will be based on "Fish". If you have time during or after the training, select another species group from page 5 to work through on the worksheet.]
      [Hint: Your answer should include records for all endpoints including those where no adverse effect was found (e.g., NOEC)!]

      ii. Filter the results to see what types of effects had calculated endpoints indicating adverse effects (e.g., LOEC, LC50 etc…) observed in the Species Group you focused on? *[Again, for this first round of the worksheet, the output will be based on "Fish". If you have time during or after the training, select another species group from page 5 to work through on the worksheet.]*

      iii. What were some of the specific effects measured?

   b. Change your results to Plot View.

      i. What were the lowest concentrations for which these effects were reported?
      [Hint: You can toggle the ⌄ in the column to switch from highest to lowest concentrations, or change the number of "Rows per page" under the output

table to see more data results.]

    ii.   What paper or papers were these lowest concentrations reported in? Copy the citation information (including the ECOREF number) by clicking on the Author(s) name in the reference column.

    iii.   Write down the ECOREF number (identifier for the reference).

c.   Select "Send Query Filters to Search" (green box) at the top of the right-hand side. This will open Search function in a new tab. *[Hint: Be sure to click the green Update Search button on the bottom-left to obtain results!]*

    i.   Modify the Publications Options to limit the output to the reference identified above. How many records are displayed?

    ii.   Use the "Customize Output Fields" feature to add fields to the output table. Select **Control** and any other output fields of interest (e.g., Gender, Experimental Design, and EE Comment). Select "Save" to update your results. What did you choose?

    iii.   Did the authors of the above paper(s) report what types of controls were used? If so, what were the types of controls?

    iv.   Were you able to find/access the publication to read/review the original results? Did you encounter challenges or have questions about the results?

d. Expand the Publications Options to include all references that meet the search parameters (no longer limiting results to the single identified reference). Now how many records are displayed?

e. Export and save the results as an Excel file and filter them to show the records from the reference with the lowest effect concentrations discussed in the previous steps. Now, try to find the same list of papers by using the Search module. Begin by adding the chemical name or CAS Registry Number and species group to the parameters on the left-hand side.

   i. Did you find that Explore or Search was an easier starting point for your query? List one example of why.

Reflection

1. In what case example from your work environment would ECOTOX be useful?

2. What have you learned about the process and workflow used to find information and papers in ECOTOX?

3. What challenges did you encounter, and how did you solve them?

Chemical List

Category	Compound(s)	Full Chemical Name	CAS Registry Number(s)
Pesticide/Herbicide	Atrazine	6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine	1912-24-9
Pesticide/Herbicide	Roundup	N-(Phosphonomethyl)glycine compd. with 2-propanamine (1:1)	38641-94-0
Pesticide/Herbicide	Chlorpyrifos	Phosphorothioic acid, O,O-Diethyl O-(3,5,6-trichloro-2-pyridinyl) ester	2921-88-2
Metal	Cadmium	-	7440-43-9, 10108-64-2, plus 11 others in the Cadmium group
Metal	Lead	-	7439-92-1, 7758-95-4, 301-04-2, 10099-74-8, plus 9 others in the Lead group
Metal	Selenium	-	35 unique compounds in the Selenium group
Pharmaceutical/Personal Care Product	17α-Ethinylestradiol	(17alpha)-19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol	57-63-6
Pharmaceutical/Personal Care Product	Clofibrate/Clofibric Acid	2-(4-Chlorophenoxy)-2-methylpropanoic acid, Ethyl ester; 2-(4-Chlorophenoxy)-2-methylpropanoic acid	637-07-0, 882-09-7
Pharmaceutical/Personal Care Product	DEET	N, N-Diethyl-meta-toluamide or diethyltoluamide	134-62-3

Species Groups

Vertebrates	Invertebrates	Plants and Other
Fish	Insects/Spiders	Flowers, Trees, Shrubs, Ferns
Mammals	Worms	Algae
Birds	Molluscs	Fungi
Amphibian	Crustaceans	Moss, Hornworts
Reptiles	Other Invertebrates	Miscellaneous (Communities, Higher Taxonomic Level)